

from physics, chemistry, biochemistry, mathematics, and statistics. This interesting blend of fields created a tower of Babel out of which evolved a communication currency based on the tools and techniques useful for computer analyses of biological data. It is thus not surprising that bioinformatics can be presented by means of a methodology thread, which is the way chosen by Pierre Baldi and Søren Brunak in their book *Bioinformatics: The Machine Learning Approach*.

The core of *Bioinformatics* is the Bayesian probabilistic framework. That focus permeates all the calculations and algorithms presented in the book and gives the book a strong sense of continuity and unity. It is conceivable that the book could have been organized in terms of such biologically important topics as protein structure prediction, sequence alignment, protein family classification, and the like. That the book is organized around techniques underscores the authors' intent: Theirs is a book on methods rather than on specific problems.

Baldi and Brunak cover an enormous amount of information. Here are some highlights: Chapter 1 includes an interesting discussion on the quality of data, and the sources of the many errors contained in the rapidly expanding biological databases. Chapter 2 sets the tone of the book in terms of how to "think" Bayesian. Examples of Bayesian inference are provided in chapter 3. An account of many important optimization techniques is the subject of chapter 4. Chapters 5 through 8 are the juiciest ones, introducing the book's main machine-learning algorithms: neural networks and hidden Markov models. These chapters also deal in detail with some of the key questions of bioinformatics, such as protein secondary structure prediction, intron-splice-site prediction, and identification of the important G-protein coupled receptors (GPCR) protein family. Chapter 9 confers additional unity to the book, as it presents neural networks and hidden Markov models in light of more general probabilistic graphical models. A brief, example-free chapter 10 deals with the inference of phylogenetic trees. Chapter 11 succinctly introduces stochastic grammars and linguistics application to RNA secondary structure prediction. Chapter 12 introduces a Bayesian hypothesis-testing scheme for gene-expression analysis in DNA microarray data and a brief summary of clustering techniques. Unfortunately no concrete biological example

illustrates this chapter. The last chapter (13) is a very useful list of public database resources that are accessible over the Internet. The book finishes with a set of six appendices that dig deeper into the technicalities of some of the subjects touched upon in the earlier chapters. Chapter 12 and appendix E (on support vector machines and Gaussian processes) are new and welcome additions to this second edition (in which many of the typos of the first edition have managed to survive, and new typos have crept in).

The authors aim at an audience of students and more advanced researchers with diverse backgrounds, who in the authors' view, do not need previous knowledge of DNA, RNA, and proteins. Such knowledge, however, seems to me to be a necessary prerequisite. I see this book as aimed at an audience with some bioinformatics experience and a desire to get deeper into a subset of methods used in the field. Readers with physics training may find some examples particularly easy to relate to, as many optimization results are presented in terms of associated free energies. Readers not acquainted with physics concepts, however, will probably not appreciate the many free-energy analogies.

The book is lucidly written. The basic algorithms are complemented with thoughtful comments drawn from the authors' considerable hands-on experience. Long passages of the book read like thorough reviews of the subject being presented and include extensive descriptions of the literature. Indeed, the reference list grew to 587, from the 452 references contained in the previous edition. The passages describing the authors' own work (including an analysis of the GPCR protein family and an analysis of symmetries of the genetic code) convey an excitement that goes beyond the pure presentation of a methodology.

Throughout the book, the authors argue that the use of priors (probabilities assigned to models that explain the data prior to our present experimentation) in Bayesian inference is a source of flexibility in the analysis. The lack of explicit priors was one of the criticisms the authors made (in chapter 3) of the traditional derivation of the Gibbs distribution in statistical mechanics. In the context of statistical mechanics, however, the use of statistical ensembles is indeed an indirect way to choose priors, except that these priors are not associated with a subjective belief but rather are dictated by the physics of the problem. In the micro canonical

ensemble, for example, Liouville's theorem tells us that the probability of each microstate is uniform. The use of conjugate priors is nicely illustrated in chapter 12, where the parameters of the posterior probability combine information from the prior probability and the data in a very meaningful way.

This is a very good book, written with a high level of erudition and insight. It provides an excellent account of the important place that machine learning plays in bioinformatics. It also constitutes a reference source of methodologies and applications for the computational biologist. And it should certainly increase the degree of belief in Bayesian inference, even for those readers without much prior experience.

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The Lattice Boltzmann Equation for Fluid Dynamics and Beyond

▶ Sauro Succi
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The Navier–Stokes equations describe the flow of simple fluids. The equations can be derived easily by applying the laws of mass conservation and Newton's second law to an elementary fluid volume ("volumelet," in the charming terminology of Sauro Succi's *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*) incorporating the assumption that stress and strain are proportional.

Despite their apparent simplicity, the Navier–Stokes equations describe rich physics, some of which is still not understood in detail. For example, at high Reynolds numbers (low viscosities, high velocities, and large length scales) flow becomes turbulent, as exemplified by waterfalls, blood flow, and atmospheric flows. In such flows, the nonlinear nature of the Navier–Stokes equations is making itself felt; many different length scales contribute to the fluid motion.

Solving the Navier–Stokes equations preoccupies many scientists and engineers. Geophysicists need to predict the flow of ocean currents, engineers designing cars aim for streamlining to reduce turbulence, and reactor physicists model flow and heat transfer under extreme conditions. For computational fluid dynamics, commercial

codes that solve the Navier–Stokes equations are well tested and widely used.

The codes are excellent for simple flow in simple geometries, but life becomes more tricky when tortuous boundaries, turbulence, or multiphase flows become important. And, of course, the investigator's goal is always to encompass ever larger systems on increasingly fine grids.

Hence the excitement when, in 1986, Uriel Frisch, Brosl Hasslacher, and Yves Pomeau proposed a lattice-gas cellular automaton able to solve two-dimensional flow. Particles hopping on a hexagonal lattice, interacting at the nodes via simple collision rules, were shown to obey the Navier–Stokes equations for sufficiently long length and time scales.

Here was a new approach to computational fluid dynamics that was free of round-off errors and ideally suited to parallel computers. But there were problems: statistical noise, a lack of Galilean invariance, and limitations to low Reynolds number.

In the Frisch-Hasslacher-Pomeau model, the particle collisions conserve mass and momentum and the hexagonal lattice has just enough symmetry to reproduce the rotational isotropy of 2D space. Essentially, the conservation laws are fed in, and the Navier–Stokes equations drop out. This idea has spurred the development of a wide range of novel Navier–Stokes solvers. Perhaps most successful of those is the lattice Boltzmann algorithm of Succi's book. The book's first few chapters give an account of the way in which lattice Boltzmann ideas developed from lattice-gas cellular automata. Succi was closely involved in those developments and one of the driving forces behind them. The evolution of the different approaches and the excitement of the research come across clearly in his book.

How does lattice Boltzmann compare to more conventional computational fluid dynamics approaches? The second part of the book discusses the technical details of irregular grids and boundary conditions and outlines applications of lattice Boltzmann algorithms to flow in porous media and to turbulence. Succi has experience with a wide range of Navier–Stokes solvers and presents a balanced view, although he is obviously fond of the lattice Boltzmann approach and pleased when it performs well. For standard applications, lattice Boltzmann is unlikely to displace more conventional methods, but for certain problems, such as multiphase flow in porous media, it is a strong contender for the

best fluid-simulation approach currently available.

The lattice Boltzmann equation can also be thought of as a discrete, simplified version of the continuum Boltzmann equation of nonequilibrium statistical mechanics. This connection has the tantalizing consequence that lattice Boltzmann may contain more mesoscopic physics than the Navier–Stokes equations themselves. For example, the lattice Boltzmann algorithm is particularly adept at describing the flow of complex fluids in which thermodynamic and hydrodynamic information comes into play.

Applications to multiphase fluids, colloids, reaction–diffusion equations, and other problems at the forefront of research, such as a lattice Boltzmann description of quantum mechanics, are summarized in the final third of the book. Inevitably, the treatment is already somewhat dated and superficial, but it provides a flavor of the possible and the exciting.

This is a book for the enthusiast that reminds the expert how much fun he can have investigating the physics and applications of this rich field.

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The Glass Transition: Relaxation Dynamics in Liquids and Disordered Materials

► E. Donth
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Ernst-Joachim Donth's *The Glass Transition* is a welcome addition to the literature on a subject that is currently attracting a very heavy research interest. Early in the book, it becomes clear that, by the title term "glass transition," the author means the entire process of viscous slowdown and vitrification. This process takes a material from the moderately viscous liquid, in which the liquid dynamics departs from the exponentially relaxing character of the "simple" liquid state, down to the rigid solid, well below the temperature known as the "normal" glass transition temperature, T_g . The study of slowdown and vitrification, often characterized by the broader description "viscous liquids and the glass transition," is currently like an Arizona brushfire, with active tongues from many previously disparate but individually active areas merging into one

large intellectual conflagration.

Donth approaches his subject from a very broad perspective; he may well be the best-read author in this field. I found information that was new and interesting to me in nearly every section of the book. There seems to be no element of the subject on which Donth has not read widely and thought deeply. We may not agree with every one of the conclusions he reaches, and—like most authors—he is capable of making errors in reporting what others have written. But there can be no doubt that he has addressed the enormous literature diligently and open-mindedly, and has drawn his own conclusions only after much intelligent reflection.

Donth has a distinct style, to which I am partial. He is an unreconstructed "figure freak." There are pages of diagrams, nearly every one of which focuses on several different elements of a given problem segment, each segment represented by its own succinct small diagram. It seems that a whole phenomenology may be represented on the single page. This use of figures, backed up by appropriate text, can be an effective way of conveying a lot of information about (and insight into) the system behavior. In some cases, though, the information provided in caption or text was too compressed for me to see the full meaning of the diagrams.

The book is divided into two main parts that deal, respectively, with phenomenological descriptions of the molecular slowdown in all its distinct aspects (chapter 2) and with theoretical approaches to interpreting these phenomena (chapters 3 and 4). There is also a brief introduction and an epilogue. The organization within the two main parts is a little convoluted, with themes being introduced in one section, and then being elaborated only later, after more descriptive background has been supplied.

While the book is comprehensive in its coverage of the phenomenology of the glass transition in the broad sense, and gives unusually detailed coverage to such little-understood phenomena as Fischer clusters and speckle phenomena, some themes are particularly stressed. A major one, not surprising in view of the work for which the author is best known, is fluctuations. The crossover point, or crossover temperature (T_c), above the glass temperature, at which the structural fluctuations change character, is given special attention. The crossover temperature is the point at which the "slow β " relaxation process usu-